

Discrete Boltzmann modeling of liquid-vapor system

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(Dated: March 18, 2014)

Abstract

We further probe the Discrete Boltzmann Modeling(DBM) of the single-component two phase flows or the liquid-vapor system. There are two kinds of nonequilibrium effects in the system. The first is the Mechanical NonEquilibrium(MNE). The second is the Thermodynamic NonEquilibrium(TNE). The MNE is well described in the traditional fluid dynamic theory. The description of TNE resorts to the gas kinetic theory. Since based on the Boltzmann equation, the DBM makes possible to analyze both the MNE and TNE. The TNE is the main discussion of this work. A major purpose of this work is to show that the DBM results can be used to confirm and/or improve the macroscopic modeling of complex system.

PACS numbers: 47.11.-j, 47.40.-x, 47.55.-t, 05.20.Dd

I. INTRODUCTION

A. Classification of LB methods

In the past two decades the Lattice Boltzmann (LB) method has been becoming a powerful simulation tool in various complex fluids[1], especially in multiphase flows, a few examples are referred to Refs.[2–11]. In most of the existing studies on LB methods and LB simulations, the LB generally appears as a kind of new numerical scheme to solve the corresponding partial differential equations. As pointed out in the early studies[1], appropriately designed LB can work as a new kind of mesoscopic kinetic model for various complex behaviors[12, 13]. In this work we refer a LB model in the second class to as a Discrete Boltzmann Model(DBM). Besides recovering the macroscopic hydrodynamic equations in the continuum limit, a DBM should present more kinetic information on the nonequilibrium effects which are generally related to some mesoscopic structures.

B. Classification of nonequilibrium behaviors

For a flow system without chemical reaction, there are two kinds of nonequilibrium behaviors, the Mechanical NonEquilibrium (MNE) and Thermodynamic NonEquilibrium (TNE). The MNE makes the acceleration, breaks the steady state, and consequently results in the further evolution of the flow system. The MNE is generally well described by the traditional fluid mechanics which is based on the continuous assumption and describes the evolution of macroscopic quantities like the density $\rho(\mathbf{r}, t)$, the momentum $\rho(\mathbf{r}, t)\mathbf{u}(\mathbf{r}, t)$ and the energy $E(\mathbf{r}, t)$, where \mathbf{r} and t are the position and time. The evolution equations of the traditional fluid mechanics appear also as the conservation laws of the mass, momentum and energy. The theory at this level do not access the behavior of the molecules. As the fundamental equation of nonequilibrium statistical physics, the Boltzmann equation describes the flow system from a more fundamental level. It resorts to the concept of distribution function $f(\mathbf{r}, \mathbf{v}, t)$, where \mathbf{v} is the molecular velocity. In the thermodynamic equilibrium state, the molecular velocity follows the Maxwellian distribution function $f^{(0)}(\mathbf{r}, \mathbf{v}, t)$. The Boltzmann equation with the BGK model reads,

$$\frac{\partial f}{\partial t} + v_\alpha \frac{\partial f}{\partial r_\alpha} + a_\alpha \frac{\partial f}{\partial v_\alpha} = -\frac{1}{\tau} (f - f^{(0)}), \quad (1)$$

where τ is the relaxation time, \mathbf{a} is an external force acting on the molecule with the unit mass, and $\alpha = x, y$. The first three low order moments of the distribution function f are related to the density ρ , momentum $\rho \mathbf{u}$ and energy $E = \frac{1}{2} \rho \mathbf{u}^2 + \rho T$ as below:

$$\begin{aligned} \int f d\mathbf{v} &= \int f^{(0)} d\mathbf{v} = \rho, \\ \int \mathbf{v} f d\mathbf{v} &= \int \mathbf{v} f^{(0)} d\mathbf{v} = \rho \mathbf{u}, \\ \int \frac{1}{2} \mathbf{v}^2 f d\mathbf{v} &= \int \frac{1}{2} \mathbf{v}^2 f^{(0)} d\mathbf{v} = \frac{1}{2} \rho \mathbf{u}^2 + \rho T, \end{aligned}$$

where \mathbf{u} and T are the local flow velocity and temperature, respectively. For the convenience of description, we use $\mathbf{M}_{m,n}(f)$ to denote the moment of f . It is a n -th order tensor in molecule velocity \mathbf{v} contracted from the m -th tensor. It is clear that $\mathbf{M}_{0,0}(f) = \mathbf{M}_{0,0}(f^{(0)}) = \rho$, $\mathbf{M}_{1,1}(f) = \mathbf{M}_{1,1}(f^{(0)}) = \rho \mathbf{u}$, $\mathbf{M}_{2,2}(f) = \mathbf{M}_{2,2}(f^{(0)}) = E$. The higher order moments are related to macroscopic quantities which are not necessarily conserved during the evolution. Besides ρ , $\rho \mathbf{u}$ and E , the Boltzmann equation is also capable of accessing non-conserved macroscopic quantities, which is the point being beyond the traditional fluid mechanics. The difference of a non-conserved macroscopic quantity, $\mathbf{M}_{m,n}(f)$, from its value in corresponding thermodynamic equilibrium, $\mathbf{M}_{m,n}(f^{(0)})$, is a kind of manifestation or measure of the TNE. For the convenience of describing the pure TNE effects, we define also the central moment $\mathbf{M}_{m,n}^*(f)$ which is the n -th order tensor in relative velocity $(\mathbf{v} - \mathbf{u})$ contracted from the m -th tensor.

C. Progress of discrete Boltzmann modeling TNE

An appropriately designed DBM should inherit partly this merit [12, 13].

The idea using DBM to access the TNE behavior [12] has been further specified and applied in various compressible flow systems via several models [14–18]. Examples of LBGK for compressible flow systems are referred to Refs. [15, 16] where preliminary studies on shock-ing behavior are shown. An example of MRT-LB for compressible flow systems is referred to Ref. [18]. In Refs. [14, 17] the TNE behaviors in combustion systems are initially investigated

via LBGK models. Up to now, all the previous studies on the discrete Boltzmann modeling of TNE behaviors were for systems following the ideal-gas equation of state.

In this work we further probe the kinetic nature of DBM for the non-ideal gas systems, particularly, the liquid-vapor system or single-component two phase flows.

II. KINETIC MODELING OF NON-IDEAL GAS SYSTEM

For the ideal gas system, $\mathbf{a} = 0$, and the local pressure $P = \rho T$. If do not consider the boundary effects, the gradient of any macroscopic quantity, for example $\nabla\rho$, $\nabla\mathbf{u}$, ∇T , or ∇P , work as a driving force for thermodynamic nonequilibrium effects. For the liquid-vapor system, the existence of the interparticle force makes the situation more complex. The force term in the LB equation is a second kind of driving force for the TNE effects. The two kinds of driving forces tend to balance each other. The competition of the two kinds of driving forces determines the evolution of the system. When the system arrives at its steady state, i.e., the mechanical equilibrium, the two kinds of driving forces balance each other.

A. Maxwellian or not in steady state?

A question here is whether or not the distribution function is the Maxwellian when the liquid-vapor system is in a steady state. We first assume and confirm it is.

In the steady state, if

$$f = f^{(0)}, \quad (2)$$

then, equation (1) requires

$$v_\alpha \frac{\partial f^{(0)}}{\partial r_\alpha} + a_\alpha \frac{\partial f^{(0)}}{\partial v_\alpha} = 0. \quad (3)$$

When the inhomogeneity exists, for example, around the interfaces,

$$\frac{\partial f^{(0)}}{\partial r_\alpha} \neq 0, \quad (4)$$

$$\frac{\partial f^{(0)}}{\partial v_\alpha} \neq 0, \quad (5)$$

the effects of the force term and the advection term balance each other. When the inhomogeneity does not exists, for example, far from the interfaces,

$$\frac{\partial f^{(0)}}{\partial r_\alpha} = 0, \quad (6)$$

$$\frac{\partial f^{(0)}}{\partial v_\alpha} \neq 0. \quad (7)$$

It is clear that the advection term makes no effects. Now, we check the force term in particle velocity derivative. In the currently using liquid-vapors models, the force a_α is from the spatial derivative of some macroscopic quantity like the pressure or density. Therefore, $a_\alpha = 0$ in the homogeneous region. Up to this step, we can confirm physically that, in the steady state, $f = f^{(0)}$.

B. Where are the meaningful nonequilibrium effects?

In the steady state, no matter far from or around the interfaces, $f = f^{(0)}$. Consequently, the total or net TNE effects

$$\Delta_{m,n} = \mathbf{M}_{m,n}(f) - \mathbf{M}_{m,n}(f^{(0)}) = \mathbf{0}. \quad (8)$$

$$\Delta_{m,n}^* = \mathbf{M}_{m,n}^*(f) - \mathbf{M}_{m,n}^*(f^{(0)}) = \mathbf{0}. \quad (9)$$

But before arriving at the steady state, $\Delta_{m,n}$ and $\Delta_{m,n}^*$ can work as measures of the TNE.

The kinetic model (1) can also be rewritten as

$$\frac{\partial f}{\partial t} + v_\alpha \frac{\partial f}{\partial r_\alpha} = -\frac{1}{\tau} (f - f^{(0)NEW}) \quad (10)$$

where

$$f^{(0)NEW} = f^{(0)} - \tau a_\alpha \frac{\partial f}{\partial v_\alpha} \quad (11)$$

can be regarded as a new equilibrium state shifted due to the existence of interparticle interactions. We define

$$\Delta_{m,n}^C = \mathbf{M}_{m,n}(f) - \mathbf{M}_{m,n}(f^{(0)NEW}), \quad (12)$$

$$\Delta_{m,n}^{*C} = \mathbf{M}_{m,n}^*(f) - \mathbf{M}_{m,n}^*(f^{(0)NEW}). \quad (13)$$

In the steady state,

$$\Delta_{m,n}^C = \mathbf{M}_{m,n}(f - f^{(0)} + \tau a_\alpha \frac{\partial f}{\partial v_\alpha}) \quad (14)$$

$$= \mathbf{M}_{m,n}(\tau a_\alpha \frac{\partial f}{\partial v_\alpha}) \quad (15)$$

$$\approx \mathbf{M}_{m,n}(\tau a_\alpha \frac{\partial f^{(0)}}{\partial v_\alpha}) \quad (16)$$

$$= \mathbf{M}_{m,n}(-\tau \frac{a_\alpha}{T}(v_\alpha - u_\alpha)f^{(0)}), \quad (17)$$

$$\begin{aligned} \Delta_{m,n}^{*C} &= \mathbf{M}_{m,n}^*(f - f^{(0)} + \tau a_\alpha \frac{\partial f}{\partial v_\alpha}) \\ &\approx \mathbf{M}_{m,n}^*(-\tau \frac{a_\alpha}{T}(v_\alpha - u_\alpha)f^{(0)}). \end{aligned}$$

It is clear that in the steady state $\Delta_{m,n}^C$ or $\Delta_{m,n}^{*C}$ (approximately) describes the TNE due to the interparticle interactions or interfacial forces. Before arriving at the steady state, it (approximately) describes the combined effects of the inhomogeneities and the interfacial forces.

C. Beyond the traditional fluid dynamics

In most studies based on the traditional fluid dynamics, the heat conduction is assumed to follow the Fourier law,

$$q = \lambda \nabla T, \quad (18)$$

and the viscous stress is assumed to follow the Newton model,

$$\boldsymbol{\sigma} = \gamma \nabla \mathbf{u}, \quad (19)$$

where the coefficients λ and γ are constants. The DBM should be capable of presenting results for checking the validity of the two assumptions and to find more reasonable responsive relations for the complex transportation processes.

The steady state is a trivial case for the LB simulation. The main purpose of the DBM is to simulate the evolution of the system before it arrives at the final steady state, and the DBM results should confirm or being helpful for improving the physical modeling from the macroscopic scale.

The relations $\Delta_{m,n}^*$ versus the gradients of macroscopic quantities ($\nabla\rho$, ∇T , $\nabla\mathbf{u}$, ∇P) show the nonequilibrium responses to nonequilibrium driving forces. From these results, the Fourier law, Newton assumption, etc., can be checked, and improved and more interesting dependences may be found.

III. DISCRETE KINETIC MODEL

In constructing the discrete Boltzmann kinetic models for non-ideal gas system, a key step is to approximate f by $f^{(0)}$ in the force term of the original BGK equation before discretizing the space of particle velocity. Since

$$\frac{\partial f}{\partial v_\alpha} \approx \frac{\partial f^{(0)}}{\partial v_\alpha} = \frac{1}{T}(v_\alpha - u_\alpha)f^{(0)} \quad (20)$$

Therefore, the currently using DBM for liquid-vapor system reads,

$$\frac{\partial f_j}{\partial t} + v_{j\alpha} \frac{\partial f_j}{\partial r_\alpha} + \frac{a_\alpha}{T}(v_{j\alpha} - u_\alpha)f_j^{(0)} = -\frac{1}{\tau} \left(f_j - f_j^{(0)} \right), \quad (21)$$

or equivalently,

$$\frac{\partial f_j}{\partial t} + v_{j\alpha} \frac{\partial f_j}{\partial r_\alpha} = -\frac{1}{\tau} \left[f_j - f_j^{(0)NEW} \right] \quad (22)$$

where the subscript “ j ” is the index of the discrete velocity and

$$f_j^{(0)NEW} = f_j^{(0)} + \tau \frac{a_\alpha}{T}(v_\alpha - u_\alpha)f_j^{(0)}. \quad (23)$$

In the steady state,

$$\Delta_{m,n}^C = \mathbf{M}_{m,n}(-\tau \frac{a_\alpha}{T}(v_\alpha - u_\alpha)f_j^{(0)}). \quad (24)$$

$$\Delta_{m,n}^{*C} = \mathbf{M}_{m,n}^*(-\tau \frac{a_\alpha}{T}(v_\alpha - u_\alpha)f_j^{(0)}). \quad (25)$$

Under the framework of DBM, in the definitions of $\mathbf{M}_{m,n}$ and $\mathbf{M}_{m,n}^*$, $\int d\mathbf{v}$ is replaced by \sum_j .

IV. CONCLUSION

We present a framework for constructing discrete Boltzmann Kinetic model for the liquid-vapor system or single-component two phase flows. Besides the mechanical nonequilibrium being well described by traditional computational fluid dynamics, the discrete Boltzmann

kinetic model can be applied to access the thermodynamic nonequilibrium behaviors. The idea presented here works also for constructing MRT-DBM for non-ideal gas systems.

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